altering individual glycosylation sites on the interaction between integrin head domains. Part of the analysis was conducted using the molecular soft docking program, BiGGER (Krippahl, 2003). Docking simulations were done using structure files generated from integrin subunit head domain entries in the Protein Data Bank (www.pdb.org). Dock assessment involved the measurement of subunit orientations based on user-defined anchor residues in the interacting subunits. Initial analysis was conducted on the Integrin αVβ3 heterodimer. The integrin αVβ3 head domain has four glycosylation sites, three for the αV beta propeller and one for the β3 A-domain. Sugar residues were iteratively removed from each of these glycosylation sites to determine their effects on integrin subunit interaction. Our results suggest the importance of glycosylation at αV N266 for the formation of the ligand binding site. Removal of these sugar residues resulted in the greatest deviation in predicted docking orientation. A ~90° rotation, counter-clockwise from the reference position, was predicted for the docking of the β3 subunit to the N266-deglycosylated αV subunit. This altered conformation is predicted to effectively destroy the ligand binding site and thus, disrupt integrin αVβ3 function.

2611-Pos Board B630

Infinitely Dilute Partial Molar Properties of Peptides and Proteins from Computer Simulation

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A detailed understanding of temperature and pressure effects on an infinitely dilute solute's conformational equilibrium requires knowledge of infinitely dilute partial molar properties. Established molecular dynamics methodologies generally have not provided a way to calculate these properties without either a loss of thermodynamic rigor, the introduction of non-unique parameters, or a loss of information about which solute conformations specifically contributed to the output values. Here we describe a method that is simple in execution and possesses none of the above disadvantages. We use it to calculate the infinitely dilute partial molar internal and kinetic energies, enthalpy, volume, isothermal compressibility, heat capacity, and thermal expansion coefficient for two proteins, pancreatic trypsin inhibitor and lysozyme. Further, we test the method's performance, in light of currently accessible simulation timescales, to precisely distinguish the thermodynamic differences between a native and denatured conformation of the trp-cage miniprotein. We conclude that those properties corresponding to fluctuating quantities (e.g., partial molar compressibility, thermal expansion coefficient, and heat capacity) will be computationally demanding to calculate precisely, but the other properties (e.g., partial molar volume and enthalpy) can be calculated with the computational power widely available to the community today. The ability to assign properties to specific conformations is a major advantage of our approach.

2612-Pos Board B631

Bayesian Inference to Discriminate Motion Models from Particle Trajectories

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Quantitative analysis of particle motion from particle tracking datasets–such as cell trajectories during embryonic development, receptor dynamics in cell membranes, and chromosome and kinetochore motions during spindle assembly–is a powerful approach to revealing the mechanism of transport in biological systems. However, inferring motion models from single-particle trajectories (SPTs) is non-trivial due to noise from both sampling limitations and heterogeneity in biological samples. We present two complementary approaches based on Bayesian inference to perform objective and automated analysis of SPTs. The first is a multiple hypothesis testing approach to determine the most likely mode of motion from mean-square displacement (MSD) curves derived from particle trajectories. This approach handles a large set of competing motion models–including diffusion, anomalous diffusion, confined diffusion, and directed motion–and determines which model is most justified by the evidence present in the available MSD curves. Because noise in MSD curves is highly correlated, we find that explicitly modeling the noise covariance matrix using multiple independent curves is essential for accurately determining model probabilities. The second approach fits raw particle trajectories with a Hidden Markov Model (HMM) to determine the most likely diffusion coefficient and velocity at each step along a trajectory, enabling the identification of transient motion states and dynamic transitions between motion models. These methods avoid overfitting by using an objective Bayesian framework to penalize model complexity and account for noise. These automated methods naturally scale to large numbers of particle trajectories, making them ideal for classifying motion in high-throughput screens of SPTs.

2613-Pos Board B632

Constitutive-Law Estimation of Bio-Filaments from their MD Simulations

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Continuum-mechanics based models have recently evolved as viable tools to efficiently simulate large deformations of bio-filaments. However, the deformations predicted from these models are highly sensitive to their underlying constitutive-law model. Unfortunately, lack of rigorous methods for identification of constitutive-law models leaves no option but to make ad hoc assumptions and crude approximations in constitutive-law models. We recently developed a novel system identification technique together with an inverse rod model that can systematically estimate the constitutive laws of bio-filaments from their discrete structure (MD) simulations; refer to [J. Appl. Mech., 79(5), p. 051005] and [Automatica 47(6), p. 1175-1182]. An attempt to apply this technique to microtubules suggests that traditionally assumed linearly elastic constitutive laws are inaccurate, and backs the claim of existence of twist-tension coupling in the microtubules. Furthermore, microtubules exhibit kinking with hysteresis supporting the hypothesis of a non-convex constitutive law.

2614-Pos Board B633

Rapid Measurements of Surface Tension from the Profile of Drops or Bubbles

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Methods that obtain surface tension (γ) from the shape of the interfacial profile provide the basis for studying films on the surface of drops and bubbles. Typical procedures iteratively adjust a number of parameters, including γ, to minimize the perpendicular distance from the profile to points calculated by numerical solution of the Young-Laplace equation. While these methods are robust, they are too slow to use feedback in experiments that maintain γ or other variables constant. Such experiments provide important quantitative information concerning the flux of surfactants to and from an interface during adsorption or collapse. We have instead developed a more rapid alternative method. An analytical expression (J.F. Padday, Nature, 1963) relates γ to the volume (V) of the cap between the apex and a point on the profile, the coordinates (x, z) of that point, and the tangential orientation (θ). The analytical expression has two unknowns: γ, and the curvature at the apex. Values of x, z, θ, and V at two or more points along the profile solve the equation, and provide γ. To improve the accuracy of the method, we developed a new algorithm to find x and z rapidly and with subpixel resolution. Summation of the conical segments between pairs of adjacent points provides V. Interpolation on a look-up table that relates x, z, V, and θ for Laplacian curves improves the accuracy of θ. The process for refining θ can also accurately determine contact angles of drops on surfaces. The replacement of an iterative procedure with an analytical expression can substantially reduce the computation required to determine γ in real time for experiments that use feedback.

2615-Pos Board B634

A Stochastic Emergence Model: Accounting for Genetic Noise in the "Scout Cell Model" of Dormancy Emergence

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According to previous studies, microbial diversity in the environment is dictated by the presence of a large seed bank that continuously shifts metabolic activity depending on the environmental conditions. Previous models for the bacteria biodiversity equilibrium fail to realistically simulate the emergence of species from a dormant metabolic state. A posit as to why these models fail is that microbes break from dormancy in a stochastic pattern caused by genomic noise within a species, creating the phenomenon of scout cells. If the environment is favorable for these scout cells, then they will have the opportunity to release exogenous proteins that will trigger the activation of other cells. By examining sequenced cultured ultra micro-bacteria (~20nm diameter) present in soils from the sample plot over two years, we created a model utilizing a total species list to suggest the statistical likelihood of stochastic emergence. The assumptions include the presence of some dormant cells in all populations; the presence of cells in a population always being available to switch metabolic states between active and inactive; and the necessity of a scout cell to survive in order to increase the likelihood of other members of its species to emerge. using this scout cell emergence model, we adjusted the best previously utilized models used to account for species non-dormant biodiversity.

Key Words: Bacteria, Diversity, Genomic Noise, Emergence Model, Dormancy, Microbial Seed Bank